Error Control

With this type of error control one can show that, for the resulting approximate solution

$$(x_j, y_j)_{j=0}^{N_{TOL}}$$

there exists a piecewise polynomial, $Z(x) \in C^1[a,b]$ such that $Z(x_j) = y_j$ for $j = 0, 1, \cdots N_{TOL}$ and for $x \in [a,b]$,

$$|Z^{'}(x) - f(x, Z)| \leq TOL.$$

This inequality can be shown to imply,

$$|y(x_j) - y_j| \leq \frac{TOL}{L}(e^{L(x_j - a)} - 1).$$

Local Error Estimates

Consider the Modified Euler Formula:

-	-	
1	1	-
	1/2	1/2

We have shown

$$
\begin{aligned}
z_j(x_j) &= y_{j-1} + \frac{h}{2}(k_1 + k_2) \\
&\quad + \left[\frac{1}{4} f^2 f_{yy} + \frac{1}{2} f f_{xy} + \frac{1}{4} f_{xx} - y^{'''}(x_j)\right] h^3 + O(h^4), \\
&= y_j + \left[\frac{1}{12} f_{yy} f^2 + \frac{1}{6} f f_{xy} + \frac{1}{12} f_{xx} - \frac{1}{6} f_{xy} - \frac{1}{6} f_y^2 f\right] h^3 + O(h^4), \\
&\equiv y_j + c(f) h^3 + O(h^4).
\end{aligned}
$$

Local Error Estimates (cont)

It then follows that the local error, LE, satisfies

$$LE = c(f)h^3 + O(h^4),$$

where $c(f)$ is a complicated function of f. There are two general strategies for estimating this LE, – the use of "step halving" and the use of a 3^{rd} order "companion formula".

Step Halving

Let $\hat{y}_j$ be the approximation to $z_j(x_j)$ computed with two steps of size $h/2$. If $c(f)$ is almost constant the we can show

$$z_j(x_j) = \hat{y}_j + 2c(f)(\frac{h}{2})^3 + O(h^4)$$

and from above

$$z_j(x_j) = y_j + c(f)h^3 + O(h^4).$$

Therefore the local error associated with $\hat{y}_j$, $\widehat{LE}$, is

$$\widehat{LE} \quad = \quad 2c(f)(\frac{h}{2})^3 + O(h^4) \quad = \frac{-1}{3}(y_j - \hat{y}_j) + O(h^4).$$

The method could then compute $\hat{y}_j, y_j$ and accept $\hat{y}_j$ only if $\frac{1}{3}|y_j - \hat{y}_j| < h\,TOL$.

Note that this strategy requires five derivative evaluations on each step and assumes that each of the components of $c(f)$ is slowly varying.

3^{rd}-Order Companion Formula

To estimate the local error associated with the Modified Euler formula consider the use of a 3-stage, 3^{rd} order Runge-Kutta formula,

$$\hat{y}_j \quad = \quad y_{j-1} + h(\hat{\omega}_1 \hat{k}_1 + \hat{\omega}_2 \hat{k}_2 + \hat{\omega}_3 \hat{k}_3) \ = z_j(x_j) + O(h^4),$$

We also have

$$y_j \quad = \quad y_{j-1} + \frac{h}{2}(k_1 + k_2) \ = z_j(x_j) - c(f)h^3 + O(h^4).$$

Subtracting these two equations we have the local error estimate,

$$est_j \equiv (\hat{y}_j - y_j) = c(f)h^3 + O(h^4).$$

3^{rd}-Order Companion Formula

Note that, for any 3^{rd} order formula, $k_1 = \hat{k}_1$ and if $\hat{\alpha}_2 = \alpha_2 = 1$ and $\hat{\beta}_{21} = \beta_{21} = 1$, we have $\hat{k}_2 = k_2$ and the cost is only three derivative evaluations per step to compute both y_j and est_j. Can one derive such a 3-stage 3^{rd} order Runge-Kutta formula ? The following tableau with $\hat{\alpha}_3 \neq 1$ defines a one-parameter family of such "companion formulas" for Modified Euler:

$$\begin{array}{c|ccc} - & - & & \\ 1 & 1 & - & \\ \hat{\alpha}_3 & \hat{\beta}_{31} & \hat{\beta}_{32} & - \\ \hline & \hat{\omega}_1 & \hat{\omega}_2 & \hat{\omega}_3 \end{array}$$

with

$$\hat{\beta}_{31} = \hat{\alpha}_3^2,\ \hat{\beta}_{32} = \hat{\alpha}_3 - \hat{\alpha}_3^2,\ \hat{\omega}_2 = \frac{(3\hat{\alpha}_3 - 2)}{6(\hat{\alpha}_3 - 1)},\ \hat{\omega}_3 = \frac{-1}{6\hat{\alpha}_3(\hat{\alpha}_3 - 1)},\ \hat{\omega}_1 = \frac{13\hat{\alpha}_3 - 1}{6\hat{\alpha}_3}.$$

Higher-Order Companion Formulas

This idea of using a "companion formula" of order $p+1$ to estimate the local error of a p^{th} order formula leads to the derivation of s-stage, order $(p, p+1)$ formula pairs with the fewest number of stages. Such formula pairs can be characterized by the tableau:

$$
\begin{array}{c|ccccc}
- & - & & & & \\
\alpha_2 & \beta_{21} & - & & & \\
\vdots & \vdots & & & & \\
\alpha_s & \beta_{s1} & \ldots & & \beta_{s,s-1} & - \\
\hline
 & \omega_1 & \omega_2 & \ldots & & \omega_s \\
 & \hat{\omega}_1 & \hat{\omega}_2 & \ldots & & \hat{\omega}_s
\end{array}
$$

Higher-Order Companion Formulas

Where

$$\begin{aligned} y_j &= y_{j-1} + h\sum_{r=1}^{s}\omega_r k_r &= z_j(x_j) - c(f)h^{p+1} + O(h^{p+2}), \\ \hat{y}_j &= y_{j-1} + h\sum_{r=1}^{s}\hat{\omega}_r k_r &= z_j(x_j) + O(h^{p+2}), \\ est_j &= (\hat{y}_j - y_j) &= c(f)h^{p+1} + O(h^{p+2}). \end{aligned}$$

This error estimate is a reliable estimate of the local error associated with the lower order (order p) formula. The following table gives the fewest number of stages required to generate formula pairs of a given order.

order pair	(2,3)	(3,4)	(4,5)	(5,6)	(6,7)
fewest stages	3	4	6	8	10

Choice of Stepsize, h

- Step is accepted only if $|est_j| < hTOL$.
- If h is too large, the step will be rejected.
- If h is too small, there will be too many steps.

The usual strategy for choosing the attempted stepsize, h, for the next step is based on 'aiming' at the largest h which will result in an accepted step on the current step. If we assume that $c(f)$ is slowly varying then,

$$|est_j| = |c(f)|h_j^{p+1} + O(h^{p+2}),$$

and on the next step attempted step, $h_{j+1} = \gamma h_j$, we want

$$|est_{j+1}| \approx TOL\ h_{j+1}.$$

Choice of h (cont)

But

$$|est_{j+1}| \approx |c(f)|(\gamma h_j)^{p+1} \quad = \gamma^{p+1}|est_j|.$$

We can then expect

$$|est_{j+1}| \approx TOL\ h_{j+1},$$

if

$$\gamma^{p+1}|est_j| \approx TOL\ (\gamma h_j),$$

which is equivalent to

$$\gamma^p|est_j| \approx TOL\ h_j.$$

Choice of h (cont)

The choice of γ to satisfy this heuristic is then,

$$\gamma = \left(\frac{TOL\ h_j}{|est_j|} \right)^{1/p}.$$

A typical step-choosing heuristic is then,

$$h_{j+1} = .9 \left(\frac{TOL\ h_j}{|est_j|} \right)^{1/p} h_j,$$

where $.9$ is a 'safety factor'. The formula works for use after a rejected step as well but must be modified slightly when round-off errors are significant (as might be the case for example when $TOL < 100\mu$).

Num. Integration - Quadrature

Basic Problem – Approximation of integrals

We will investigate methods for computing an approximation to the definite integral:

$$I(f) \equiv \int_a^b f(x)dx.$$

The obvious generic approach is to approximate the integrand $f(x)$ on the interval $[a, b]$ by a function that can be integrated exactly (such as a polynomial) and then take the integral of the approximating function to be an approximation to $I(f)$.

Interpolatory Rules

When an interpolating polynomial, $P_n(x)$,is used the corresponding approximation $I(P_n(x))$ is called an interpolatory rule, Consider writing $P_n(x)$ in Lagrange form,

$$P_n(x) = \sum_{i=0}^{n} f(x_i) l_i(x),$$

where $l_i(x)$ is defined by

$$l_i(x) = \prod_{j=0, j\neq i}^{n} \left(\frac{x - x_j}{x_i - x_j} \right).$$

We then have

$$\begin{aligned} \int_a^b P_n(x)dx &= \int_a^b \sum_{i=0}^{n} f(x_i) l_i(x) dx \\ &= \sum_{i=0}^{n} f(x_i) \int_a^b l_i(x) dx \equiv \sum_{i=0}^{n} \omega_i f(x_i). \end{aligned}$$

Observations

- The 'weights' (the ω_i's) depend only on the interval (the value of a and b) and on the x_i's. In particular these weights are independent of the integrand.
- The interpolatory rules then approximate $I(f)$ by a linear combination of sampled integrand evaluations.
- If $a = x_0 < x_1 < \cdots x_n = b$ are equally spaced the corresponding interpolatory rule is called a Newton-Coates quadrature rule.

Errors in Interpolatory Rules

The error associated with an interpolatory rule is $E(f) = I(f) - I(P_n)$ and satisfies,

$$\begin{aligned} E(f) &= \int_a^b f(x)dx - \int_a^b P_n(x)dx = \int_a^b [f(x) - P_n(x)]dx, \\ &= \int_a^b E_n(x)dx, \end{aligned}$$

where $E_n(x)$ is the error in polynomial interpolation and satisfies,

$$\begin{aligned} E_n(x) &= (x - x_0)(x - x_1) \cdots (x - x_n) f[x_0 x_1 \cdots x_n x], \\ &= \Pi_n(x) f[x_0 x_1 \cdots x_n x]. \end{aligned}$$

In some special cases we can simplify this expression to obtain estimates and/or more insight into the behaviour of the error.

Error Analysis - Special Cases

- First special case – If $\Pi_n(x)$ is of one sign (on $[a, b]$) then the Mean Value Theorem for Integrals implies,

$$\begin{aligned} E(f) &= \int_a^b f[x_0 x_1 \cdots x_n x]\Pi_n(x)dx, \\ &= f[x_0 x_1 \cdots x_n \xi] \int_a^b \Pi_n(x)dx, \end{aligned}$$

for some $\xi \in [a, b]$. Also since $f[x_0 x_1 \cdots x_n \xi] = \frac{f^{n+1}(\eta)}{(n+1)!}$ for some $\eta \in (a, b)$, we have shown that if $\Pi_n(x)$ is of one sign then,

$$\boxed{E(f) = \frac{1}{(n+1)!} f^{n+1}(\eta) \int_a^b \Pi_n(x)dx}$$

Error Analysis - Special Cases

Second special case – If $\int_a^b \Pi_n(x)dx = 0$ we have, for arbitrary x_{n+1},

$$f[x_0x_1\cdots x_nx] = f[x_0x_1\cdots x_nx_{n+1}] + f[x_0x_1\cdots x_{n+1}x](x - x_{n+1}),$$

and therefore,

$$\begin{aligned} E(F) &= \int_a^b f[x_0x_1\cdots x_nx]\Pi_n(x)dx, \\ &= \int_a^b f[x_0x_1\cdots x_{n+1}]\Pi_n(x)dx + \int_a^b f[x_0x_1\cdots x_{n+1}x]\Pi_{n+1}(x)dx, \\ &= \int_a^b f[x_0x_1\cdots x_{n+1}x]\Pi_{n+1}(x)dx. \end{aligned}$$

As a result, if $\int_a^b \Pi_n(x)dx = 0$ and we can choose x_{n+1} so that $\Pi_{n+1}(x)$ is of one sign, then using a similar argument as for the first special case, it follows that, if $\int_a^b \Pi_n(x)dx = 0$ and $\Pi_{n+1}(x)$ is of one sign,

$$\boxed{E(f) = \frac{1}{(n+2)!} f^{n+2}(\eta) \int_a^b \Pi_{n+1}(x)dx}$$